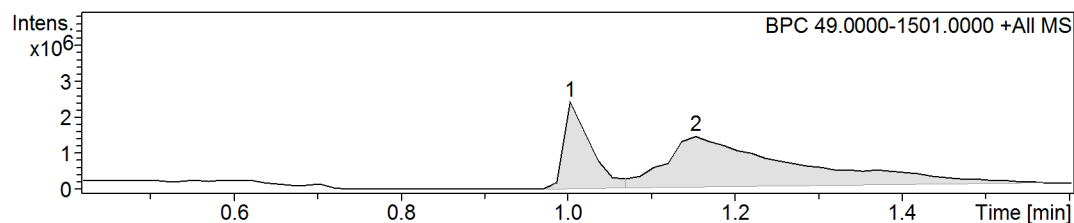


School of Chemistry Mass Spectrometry Service

SampleID JF4-512
Sample Description
Analysis Name D:\Data\michaelehardie\cmjmf\JF4-512_193988_BB5_01_31073.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

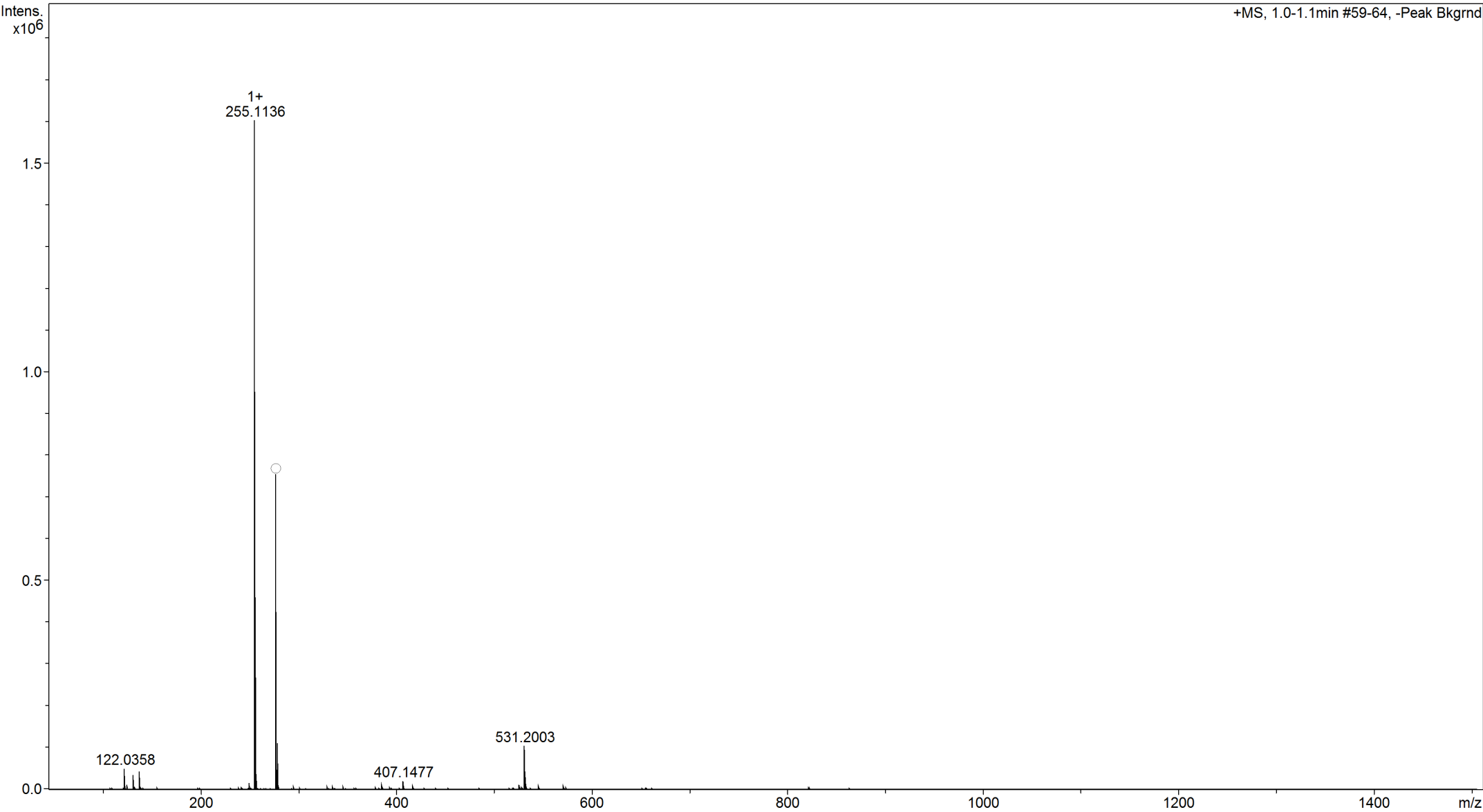
Submitter Jonathan Fowler
Supervisor Michaele Hardie
Acquisition Date 15/02/2017 09:00:54
Scan Begin 50 m/z **Scan End** 1500 m/z

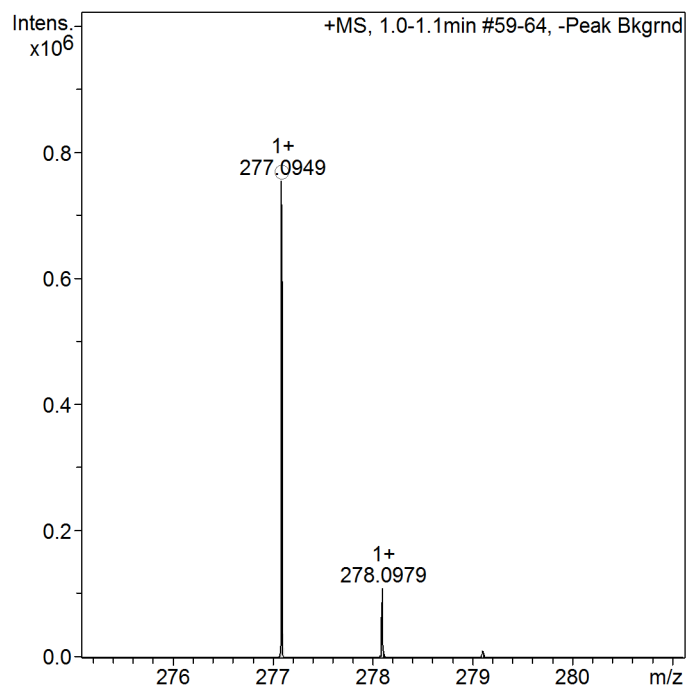


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.0 min	1.00	25.6	no uv	
Cmpd 2, 1.2 min	1.15	74.4	no uv	

Cmpd 1, 1.0 min





Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Cmpd 1, 1.0 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
277.094899	C15H14N2NaO2	1+	277.094748	0.2	0.5	15.3	100.00	C15 H13 N2 Na O2	M+H
	C15H14N2NaO2	1+	277.094748	0.2	0.5	15.3	100.00	C15 H10 N Na O2	M+NH4
	C15H14N2NaO2	1+	277.094748	0.2	0.5	15.3	100.00	C15 H14 N2 O2	M+Na
	C12H18KN2O3	1+	277.094901	-0.0	-0.0	37.9	100.00	C12 H18 N2 O3	M+K

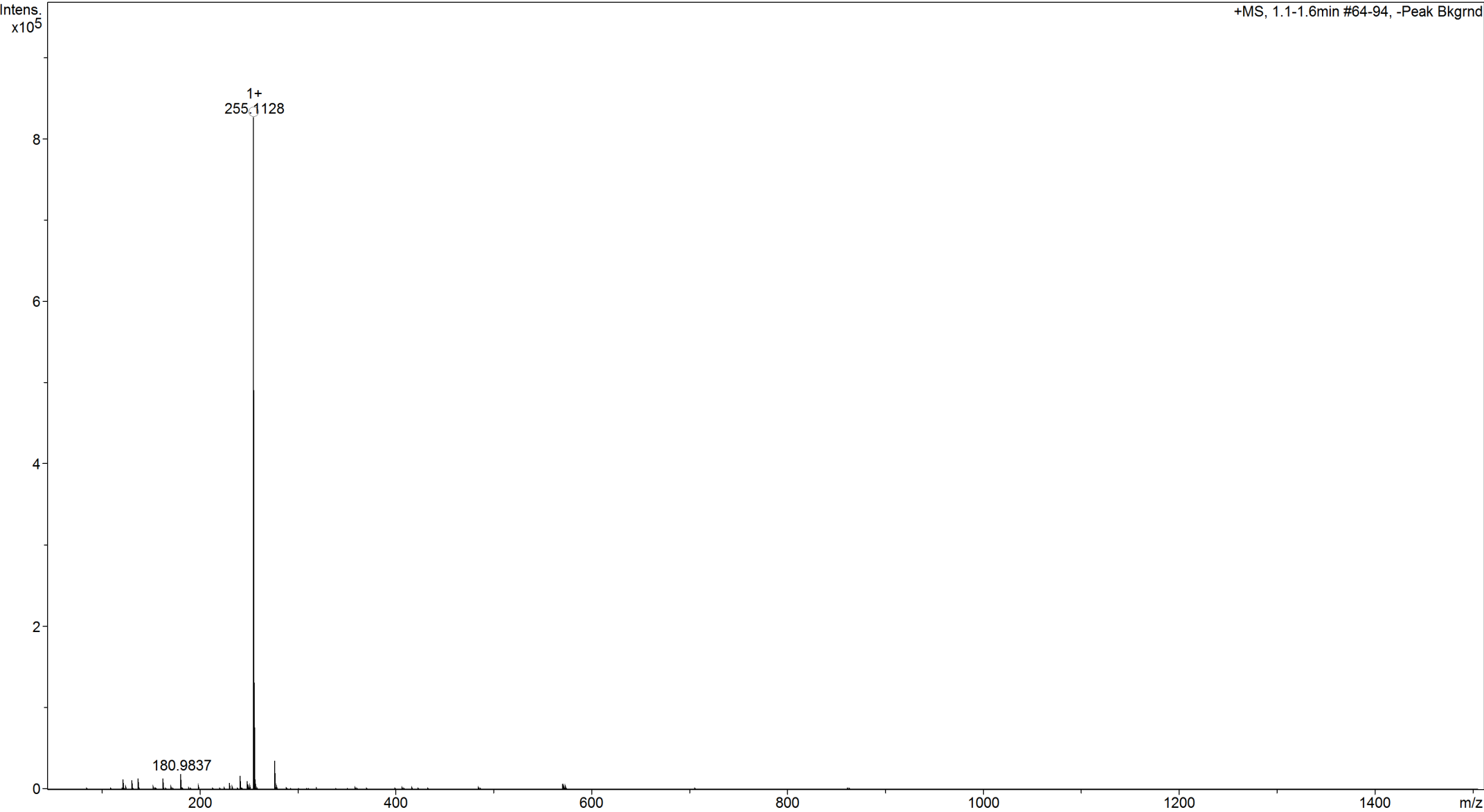
Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

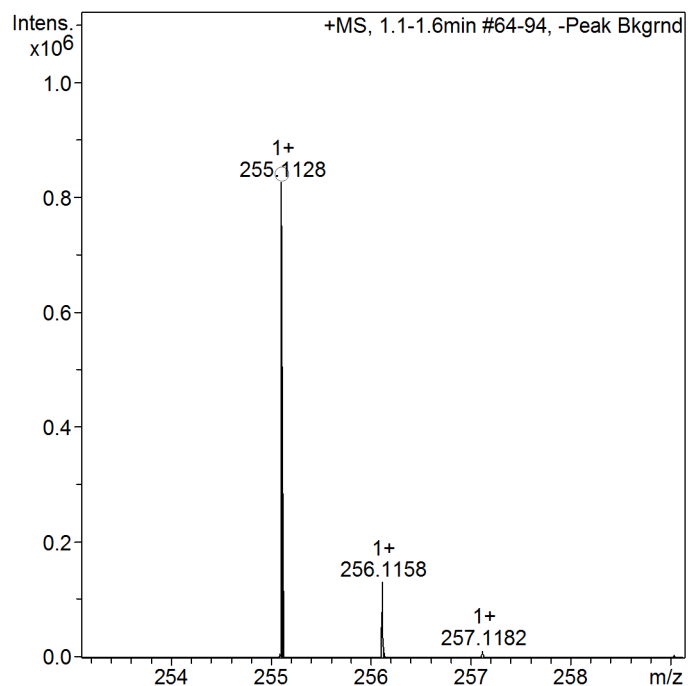
Smart Formula Search Parameters
CHNO and adducts considered
implicitly

Formula Search Minimum
Formula Search Maximum

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80

Cmpd 2, 1.2 min





Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Cmpd 2, 1.2 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
255.112848	C15H15N2O2	1+	255.112804	0.0	0.2	8.2	100.00	C15 H14 N2 O2	M+H
	C15H15N2O2	1+	255.112804	0.0	0.2	8.2	100.00	C15 H11 N O2	M+NH4
	C16H17Na2	1+	255.112016	-0.8	-3.3	9.7	100.00	C16 H18	M+Na2-H
	C16H17Na2	1+	255.112016	-0.8	-3.3	9.7	100.00	C8 H8 Na	2M+H

Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

Smart Formula Search Parameters
CHNO and adducts considered
implicitly

Formula Search Minimum
Formula Search Maximum

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80